ARNOLDI REDUCTION METHOD FOR SIMULATION OF MULTI-SPECIES CONTAMINANT TRANSPORT IN DISCRETELY FRACTURED MEDIA

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We have extended the Arnoldi reduction method (ARM) for the simulation of multispecies contaminant transport in fractured media using a discrete fracture approach. This particular class of problems can easily introduce hundreds of thousand to millions of unknowns, because a system of ordinary differential equations must be solved for each species, simultaneously with the others. The Arnoldi reduction technique uses orthogonal matrix transformations to reduce each of the aforementioned coupled systems to much smaller size. In this study, there are several improvements that have been implemented to the standard Arnoldi algorithm. One of these is to improve the convergence of the Arnoldi system itself; namely find ways to require fewer modes, or fewer Arnoldi vectors to be generated to achieve the same level of accuracy. The second of these is to use iterative, instead of direct solvers, for fractured media cases. The computational efficiency of the Arnoldi algorithm is enhanced by introducing an eigenvalue shift technique. This approach greatly improves the diagonal dominant properties of the matrices to be solved. The use of eigenvalue shift technique greatly relaxes the grid Peclet restrictions. Courant number criteria restrictions are also effectively removed. Additionally, we developed an iterative version of the Arnoldi algorithm, in which the preconditioned conjugate gradient (PCG) solver, based on ORTHOMIN acceleration, is employed within the Arnoldi reduction process. The proposed numerical method has been verified by comparison against analytical solutions. The developed model is highly efficiency in computing time and storage space. Simulations of radioactive decay chain and TCE transport are made and compared to the Laplace Transform Galerkin (LTG) method. Examples with about one million unknowns are solved on personal computers and show that the ARM is even more efficient than the LTG method, by allowing for similar speed increases with multicomponents. Therefore, the Arnoldi approach will allow for a variety complex, high-resolution problems to be solved for on small computer platforms.